Institute for Advanced Sustainability Studies (IASS)

Understanding Ozone Pollution:

A Comparison of Chemical Mechanisms

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Motivation

- Compare different representations of O_3 chemistry used in chemical transport models.
- Determine effects on O_3 production by comparing treatment of Volatile Organic Compounds (VOCs) degradation products.
- Importance of O_3 production chemistry representation – future emission scenarios.

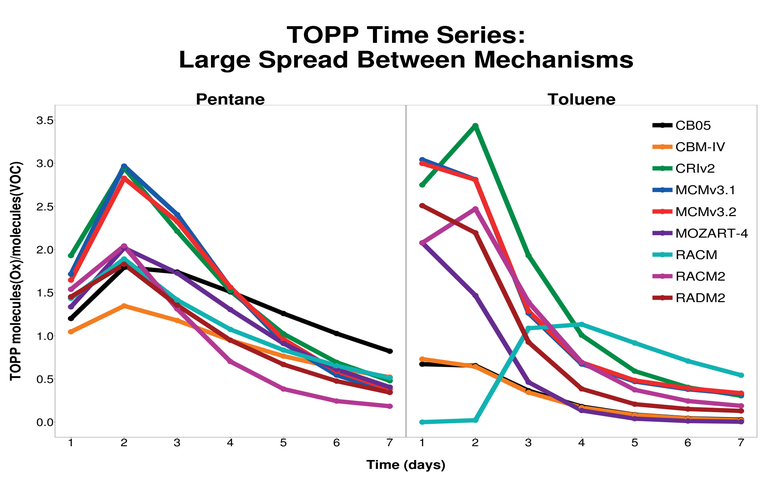
Approach

- Tagged Ozone Production Potentials (TOPPs) [1] calculated over 7 days for VOCs common to urban environments.
- Following mechanisms are compared. MCM v3.2 is the reference mechanism.

MCM v3.2	MCM v3.1	CRI v2
RADM2	RACM	RACM2
MOZART-4	CBM-IV	CB05

- O_x (= $O_3 + NO_2$) production is allocated back to the emitted VOC by tagging all organic degradation products produced from the VOC. This is done by labelling the organic products with the emitted VOC's name.
- Daily O_x production normalised by the VOC emission giving the ratio of O_x production per molecule of VOC (TOPP).

Results



Conclusions

- More explicit mechanisms show larger O_x production than those with a more streamlined approach. As VOCs break down quicker in less-explicit mechanisms, there is less O_3 produced.
- Aromatic chemistry is represented very differently between the mechanisms, resulting in a wide spread of TOPP values between the mechanisms. This is not so surprising as aromatic chemistry is not fully understood and subject to very large uncertainties in the overall chemistry. The approach taken by the RACM mechanism, in particular, differs substantially from all the other mechanisms resulting in the unrealistic net consumption of O_x on the first two days.
- The first day TOPPs are similar for a number of VOCs however there are more differences when looking at their temporal profile.

References

[1] T. M. Butler, M. G. Lawrence, D. Taraborrelli, and J. Lelieveld. Multi-day ozone production potential of volatile organic compounds calculated with a tagging approach. Atmospheric Environment, 45(24):4082–4090, 2011.

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